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A NOTE ON THE GENERALIZED CONJUGATE GRADIENT METHOD. (U)
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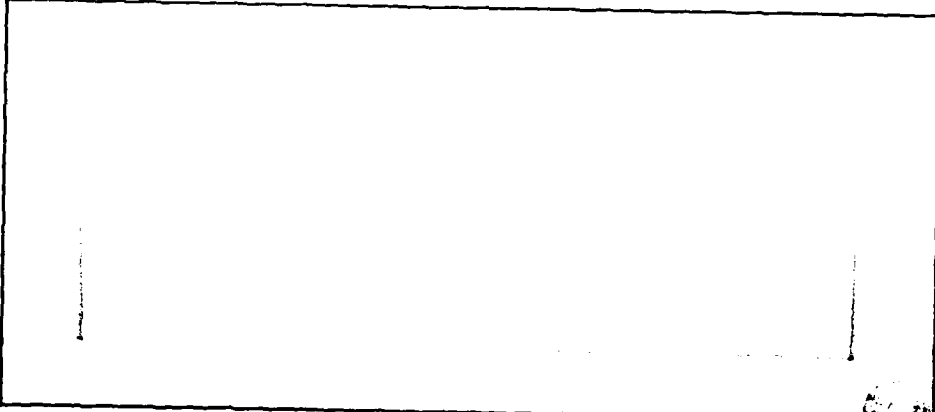
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Abstract

Each iterate generated by the Generalized Conjugate Gradient Method of Concus and Golub [1] and Widlund [3] is shown to be the best approximation to the solution from a certain affine subspace (although not from the "natural" affine Krylov subspace). This property is used to improve the error bounds given by Widlund [3] and Hageman, Luk, and Young [2].

A Note on the Generalized Conjugate Gradient Method

Stanley C. Eisenstat

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1. Introduction

The Generalized Conjugate Gradient Method of Concus and Golub [1] and Widlund [3] is an iterative method for solving a system of linear equations $Ax = b$ when the coefficient matrix A is real and has positive definite symmetric part $M = (A + A^t)/2$:

LET $x^{(0)}$ BE GIVEN AND SET $x^{(-1)} = 0$.

FOR $m = 0$ STEP 1 UNTIL "CONVERGENCE" DO

SOLVE $Mv^{(m)} = b - Ax^{(m)}$

COMPUTE¹ $\rho_m = (Mv^{(m)}, v^{(m)})$

IF $m = 0$ THEN

SET $\omega_{m+1} = 1$

ELSE

COMPUTE $\omega_{m+1} = [1 + \rho_m / (\rho_{m-1} \omega_m)]^{-1}$

COMPUTE $x^{(m+1)} = x^{(m-1)} + \omega_{m+1} (v^{(m)} + x^{(m)} - x^{(m-1)})$

Let $A = M - N$, whence $-N = (A - A^t)/2$ is the skew-symmetric part of A , and let $K = M^{-1}N$. Then it can be shown that the iterate $x^{(m)}$ lies in the affine Krylov subspace

$$x^{(0)} + \text{Span}\{v^{(0)}, Kv^{(0)}, K^2v^{(0)}, \dots, K^{m-1}v^{(0)}\} \equiv x^{(0)} + S_m$$

and is characterized by the Galerkin condition

$$(z, Ae^{(m)}) = 0 \quad \text{for all } z \in S_m, \quad (1.1)$$

where $e^{(m)} \equiv x^{(m)} - x$ (see [3]). Moreover,

$$x^{(m)} = x + p_m(K)e^{(0)} \quad (1.2)$$

where $p_m(\mu)$ is an even (odd) polynomial of degree at most m for m even (odd) and $p_m(1) = 1$ (see [3]).

In this paper, we show that $x^{(m)}$ is the *best* approximation to x from a certain m -dimensional affine subspace (but *not* from the affine Krylov subspace $x^{(0)} + S_m$) and use this property to improve the error bounds given by Widlund [3] and Hageman, Luk, and Young [2].

¹ (y, z) denotes the Euclidean inner-product.

Notation: $(y, z)_M$ denotes the M -inner product (My, z) and $\|z\|_M$ denotes the corresponding norm. Note that

$$(Ky, z)_M = (Ny, z) = -(y, Nz) = -(My, M^{-1}Nz) = -(y, Kz)_M$$

so that K is skew-symmetric with respect to $(\cdot, \cdot)_M$ and $(Kz, z)_M = 0$ for all z .

2. An Alternative Characterization

In this section, we show that the iterate $x^{(m)}$ generated by the Generalized Conjugate Gradient Method is the best approximation to x with respect to a certain m -dimensional affine subspace, but not with respect to the affine Krylov subspace $x^{(0)} + S_m$ (unless $x^{(m)} = x$). The cases m even ($= 2k$) and m odd ($= 2k+1$) are treated separately.

Theorem 2.1: $x^{(2k)} \in x^{(0)} + (I+K)S_{2k}$ and

$$(z, x^{(2k)} - x)_M = 0 \quad \text{for all } z \in (I+K)S_{2k},$$

whence

$$\|x^{(2k)} - x\|_M = \min \{ \|y - x\|_M \mid y \in x^{(0)} + (I+K)S_{2k} \}.$$

Proof:

Since $p_{2k}(-1) = p_{2k}(1) = 1$ (recall that p_{2k} is even), $p_{2k}(\mu)$ can be written in the form

$$p_{2k}(\mu) = 1 + (1+\mu) \pi_{2k-2}(\mu) (1-\mu)$$

where $\pi_{2k-2}(\mu)$ is a polynomial of degree at most $2k-2$. Therefore, by (1.2),

$$\begin{aligned} x^{(2k)} &= x + e^{(0)} + (I+K) \pi_{2k-2}(K) (I-K)e^{(0)} \\ &= x^{(0)} - (I+K) \pi_{2k-2}(K)v^{(0)} \\ &\in x^{(0)} + (I+K)S_{2k}. \end{aligned}$$

If $z \in (I+K)S_{2k}$, then $z = (I+K)u$ for some $u \in S_{2k}$ and

$$(z, x^{(2k)} - x)_M = (M(I+K)u, e^{(2k)}) = (u, Ae^{(2k)}) = 0$$

by the Galerkin condition (1.1). □

However, $x^{(2k)}$ is not the best approximation to x from $x^{(0)} + S_{2k}$. To see this, note that

$$\begin{aligned} (v^{(0)}, x^{(2k)} - x)_M &= -((I-K)c^{(0)}, c^{(2k)})_M \\ &= -(c^{(2k)}, c^{(2k)})_M + (c^{(2k)} - c^{(0)}, c^{(2k)})_M + (Kc^{(0)}, p_{2k}(K)c^{(0)})_M. \end{aligned}$$

By Theorem 2.1, $c^{(2k)} - c^{(0)} = x^{(2k)} - x^{(0)} \in (I+K)S_{2k}$ and the second term vanishes. Since K is skew-symmetric with respect to $(\cdot, \cdot)_M$ and p_{2k} is even, the third term also vanishes. Therefore, $v^{(0)} \in S_{2k}$ but

$$(v^{(0)}, x^{(2k)} - x)_M = -(c^{(2k)}, c^{(2k)})_M \neq 0,$$

unless $x^{(2k)} = x$.

Theorem 2.2: $x^{(2k+1)} \in x^{(0)} + v^{(0)} + (I+K)S_{2k+1}$ and

$$(z, x^{(2k+1)} - x)_M = 0 \quad \text{for all } z \in (I+K)S_{2k+1},$$

whence

$$\|x^{(2k+1)} - x\|_M = \min \{ \|y - x\|_M \mid y \in x^{(0)} + v^{(0)} + (I+K)S_{2k+1} \}.$$

Proof:

Since $p_{2k+1}(1) = 1$ and $p_{2k+1}(-1) = -p_{2k+1}(1) = -1$ (recall that p_{2k+1} is odd), $p_{2k+1}(\mu)$ can be written in the form

$$p_{2k+1}(\mu) = \mu + (1+\mu) \pi_{2k-1}(\mu) (1-\mu)$$

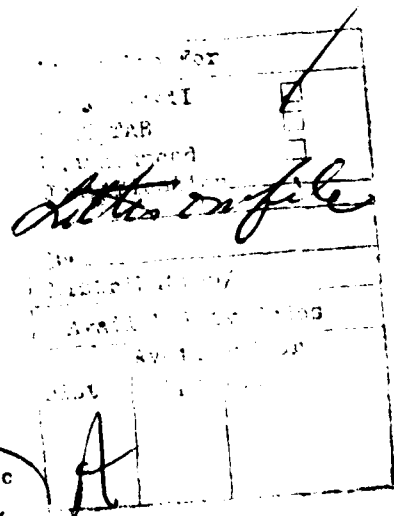
where $\pi_{2k-1}(\mu)$ is an odd polynomial of degree at most $2k-1$. Therefore, by (1.2),

$$\begin{aligned} x^{(2k+1)} &= x + Kc^{(0)} + (I+K) \pi_{2k-1}(K) (I-K)c^{(0)} \\ &= x^{(0)} - (I-K)c^{(0)} - (I+K) \pi_{2k-1}(K)v^{(0)} \\ &= x^{(0)} + v^{(0)} - (I+K) \pi_{2k-1}(K)v^{(0)} \\ &\in x^{(0)} + v^{(0)} + (I+K)S_{2k+1}. \end{aligned}$$

If $z \in (I+K)S_{2k+1}$, then $z = (I+K)u$ for some $u \in S_{2k+1}$ and

$$(z, x^{(2k+1)} - x)_M = (M(I+K)u, c^{(2k+1)}) = (u, Ac^{(2k+1)}) = 0$$

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by the Galerkin condition (1.1). □

Again, $x^{(2k+1)}$ is not the best approximation to x from $x^{(0)} + S_{2k+1}$. To see this, note that

$$\begin{aligned} (v^{(0)}, x^{(2k+1)} - x)_M &= -((I-K)e^{(0)}, e^{(2k+1)})_M \\ &= (e^{(2k+1)}, e^{(2k+1)})_M - (e^{(2k+1)} - Ke^{(0)}, e^{(2k+1)})_M \\ &\quad - (e^{(0)}, p_{2k+1}(K)e^{(0)})_M. \end{aligned}$$

By Theorem 2.2, $e^{(2k+1)} - Ke^{(0)} = x^{(2k+1)} - x^{(0)} - v^{(0)} \in (I+K)S_{2k}$ and the second term vanishes. Since K is skew-symmetric with respect to $(\cdot, \cdot)_M$ and p_{2k+1} is odd, the third term also vanishes. Therefore, $v^{(0)} \in S_{2k+1}$ but

$$(v^{(0)}, x^{(2k+1)} - x)_M = (e^{(2k+1)}, e^{(2k+1)})_M \neq 0,$$

unless $x^{(2k+1)} = x$.

3. Error Bounds

In this section, we use the best approximation property of the iterates $\{x^{(m)}\}$ to prove error bounds for the Generalized Conjugate Gradient Method.

Theorem 3.1:

$$\|x^{(m)} - x\|_M \leq \|q_m(K)(x^{(0)} - x)\|_M$$

for any real polynomial $q_m(\mu)$ of degree at most m satisfying $q_m(1) = 1$ and $q_m(-1) = (-1)^m$.

Proof:

Let $y = x + q_m(K)e^{(0)}$. Then it can be shown that $y \in x^{(0)} + (I+K)S_m$ if m is even (see the first part of the proof of Theorem 2.1) and that $y \in x^{(0)} + v^{(0)} + (I+K)S_m$ if m is odd (see the first part of the proof of Theorem 2.2). Therefore, using either Theorem 2.1 or Theorem 2.2,

$$\|x^{(m)} - x\|_M \leq \|y - x\|_M = \|q_m(K)(x^{(0)} - x)\|_M.$$

□

Let $\sigma(K)$ denote the spectrum of K . Since K is skew-symmetric with respect to $(\cdot, \cdot)_M$, it can be shown that

$$\operatorname{Re} \mu = 0, \quad |\operatorname{Im} \mu| \leq \|K\|_M = A$$

for any $\mu \in \sigma(K)$, and that

$$\|q_m(K)\|_M = \max_{\mu \in \sigma(K)} |q_m(\mu)|$$

for any real polynomial $q_m(\mu)$.

Corollary 3.2:

$$\|x^{(m)} - x\|_M \leq \frac{2}{R(A)^m + [-R(A)]^{-m}} \|x^{(0)} - x\|_M$$

where $R(A) = A^{-1} + \sqrt{A^{-2} + 1}$.

Proof:

Let $q_m(\mu) = T_m(iA^{-1}\mu)/T_m(iA^{-1})$ where $T_m(z)$ is the m^{th} Chebyshev polynomial. Since $T_m(z)$ is even (odd) when m is even (odd), $q_m(\mu)$ is a real polynomial which satisfies the conditions of Theorem 3.1 so that

$$\|x^{(m)} - x\|_M \leq \|q_m(K)(x^{(0)} - x)\|_M \leq \|q_m(K)\|_M \|x^{(0)} - x\|_M$$

But

$$\|q_m(K)\|_M = \max_{\mu \in \sigma(K)} \frac{|T_m(iA^{-1}\mu)|}{|T_m(iA^{-1})|} \leq \frac{1}{|T_m(iA^{-1})|}$$

since $-1 \leq iA^{-1}\mu \leq +1$ for all $\mu \in \sigma(K)$ and $|T_m(z)| \leq 1$ for $-1 \leq z \leq +1$. Moreover, it can be shown that

$$T_m(iA^{-1}) = \frac{i^m}{2} [R(A)^m + [-R(A)]^{-m}]$$

Therefore, since $R(A) > 1$,

$$\|x^{(m)} - x\|_M \leq \frac{2}{R(A)^m + [-R(A)]^{-m}} \|x^{(0)} - x\|_M$$

□

Hageman, Luk, and Young [2] proved Corollary 3.2 for m even by observing that the even iterates can also be generated by applying conjugate gradient acceleration to a certain

symmetrizable "double" method. Widlund [3] proved somewhat weaker bounds for general m using a standard argument for Galerkin methods.

The best approximation property and the nesting of the subspaces $\{S_m\}$ guarantees that $\{\|e^{(2k)}\|_M\}$ and $\{\|e^{(2k+1)}\|_M\}$ are both monotone decreasing. Widlund [3] gives a direct proof. The following result shows that both sequences must converge at the same rate, contradicting the experimental results reported in [3].

Corollary 3.3:

$$\Lambda^{-1} \|x^{(m+1)} - x\|_M \leq \|x^{(m)} - x\|_M \leq \Lambda \|x^{(m-1)} - x\|_M \quad \text{for all } m \geq 1.$$

Proof:

It suffices to prove the right-hand inequality. Since $q_m(\mu) = \mu p_{m-1}(\mu)$ satisfies the conditions of Theorem 3.1,

$$\begin{aligned} \|x^{(m)} - x\|_M &\leq \|q_m(K)(x^{(0)} - x)\|_M \\ &\leq \|K\|_M \|p_{m-1}(K)e^{(0)}\|_M \\ &= \Lambda \|x^{(m-1)} - x\|_M. \end{aligned}$$

□

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